AD-A280 929

FINAL REPORT

OPTICAL PROPERTIES OF SEMICONDUCTOR SUPERLATTICES

In support of

OPTICAL SENSOR SURVIVABILITY PROGRAM
Naval Research Laboratory
Washington, D. C. 20375-5000

Two Year Proposal : 7/1/91-6/30/93
extended to June 1994

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Final Report

The theoretical research performed under the auspices of this grant has played a central role in the investigation of optical and magneto-optical properties of semiconductor heterostructures.

There are two major developments to report. One is that the method of finite elements has been proved to be a very effective, flexible, and powerful approach for the calculation of energy levels in semicoductor superlattices and quantum well structures. The second is the method of tight-binding which provides a full Brillouin-zone description of the energy bands of superlattices and quantum wells.

These two approaches have allowed new theoretical insights in understanding the electronic and optical properties of heterostructures. The following items describe these new developments based on work supported by the research grant.

- The presence of quasibound states in an asymmetrical quantum well has been discussed for the first time in [1]. It is only in symmetric quantum wells that we must have at least one bound state. This theorem is no longer true in asymmetric wells. The absence of any bound state in wells narrow enough to expell all of them was verified experimentally by growing quantum wells with compositionally asymmetric barriers on either sides; the growth conditions were specified by theory before the heterostructures were grown [3].

- The finite element and transfer matrix analysis has been used for II-VI heterostructures [2].

- Above the barrier in quantum wells or above single/double barrier heterostructures there exist a continuum of states of al' ¬nergies. However, certain of these states correspond to a localization of the carrier above the barrier. This rather non-intuitive picture is easily understood once we consider the possibility of Fabry-Perot like interference effects for the wavefunctions. Experimentally, this localization has been observed in superlattices as well as above single barriers. This has been verified using the tight-binding calculations for GaAs/AlAs superlattices in which the X-like states form their own localization [8]. A study of HgTe/CdTe superlattices [9] shows that similar localization will occur in these II-VI superlattices as well.

- The transfer matrix and finite element approaches have provided a detailed understanding of the band-structure of zero-gap superlattices of HgTe/CdTe, and the rather complex magneto-optical properties have been thoroughly investigated in collaboration with the research group of Drs. Meyer and Bartoli at NRL. The inclusion of mass variation throughout the superlattice Brillouin zone, the inclusion of interband as well as intraband transitions (a distinction no longer clear cut in zero-gap superlattices), and the allowance for band variations with magnetic fields has led to the prediction of a metallic behavior in these superlattices at high fields [5,6,7].

- Our tight-binding theory has emphasised the importance of having parameters in the theory which can reproduce not only the correct energy bandgaps at special points in

the Brillouin zone of the bulk semiconductors, but also the correct band curvatures at these points. This is very critical when one uses these same parameters in semiconductor heterostructures. A Ph.D. thesis has been completed on the application of the tight-binding models to semiconductor heterostructures. One of the special results has been the derivation of a self-consistent approach, using the Feynman-Hellmann theorem, to the calculation of optical matrix elements. This has provided a new criterion for the selection of the tight-binding parameters. It has also demonstrated that the higher conduction bands need to be reproduced properly before the tight-binding parameters can be used to reliably derive the dielectric function as well as the second order optical nonlinearity in bulk III-V semiconductors [10, 23, Thesis].

- Experiments performed at NRL have shown that there are alternatives to the HgCdTe system in the InAs/GaInSb system [13, 14, 16] for band tailoring in the narrow gap regime. The analysis of the data from these experiments were again performed using the 8-band $k \cdot p$ model for heterostructures developed by me.

- Superlattice miniband formation should lead to transitions at $q = 0$ as well as at $q = 1$, where the wavevector along the growth direction in superlattices q has the units $\pi/(d_1 + d_2)$. There have been no experiments unambiguously displaying such transitions before the work done at Purdue using piezomodulation [11], in the GaAs system. The theoretical analysis demonstrates the clean solutions put out by the finite-element methods which are in excellent agreement with these experiments.

- The tight-binding model has permitted the taking into consideration the presence of subsidiary minima (such as at the X point) in the Brillouin zone. I have done feasibility studies to show that band to band lasing is possible in GaAs/AlAs short-period superlattices [18]. This calculation shows that the tight-binding methods as developed by us can be used with advantage in developing new heterostructures and understanding their device potential.

Dr. L. R. Ram-Mohan:

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1991-1994

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3. "Piezomodulated reflectivity of $Al_{x_1}Ga_{1-x_1}As/GaAs/Al_{x_2}Ga_{1-x_2}As$ asymmetric and symmetric single quantum wells"; C. Parks, R. G. Alonso, A. K. Ramdas, L. R. Ram-Mohan, D. Dossa, and M. R. Melloch, *Physical Review B* **45**, 14215-14224 (1992).

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23. "Second order nonlinear optical interaction in asymmetric semiconductor heterostructures"; L. C. Lew Yan Voon and L. R. Ram-Mohan, submitted for publication (1994).

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